A robust shock-capturing scheme based on rotated Riemann solvers

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Abstract

This paper presents a robust finite volume shock-capturing scheme based on the rotated approximate Riemann solver. A general framework for constructing the rotated Riemann solver is described and a rotated Roe scheme is discussed in detail. It is found that the robustness of the rotated shock-capturing scheme is closely related to the way in which the direction of upwind differencing is determined. When the upwind direction is determined by the velocity-difference vector, the rotated Roe scheme demonstrates a robust shock-capturing capability and the shock instabilities or carbuncle phenomena can be eliminated completely. The dissipation property associated with the linear field of the rotated flux-difference splitting scheme is analyzed, and several test cases are presented to validate the proposed scheme.

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1. Introduction

The numerical solution of systems of hyperbolic conservation laws has been dominated by Riemann-solver-based schemes since the work of Godunov [7], Van Leer [27], Harten and Lax [10], and Roe [20]. This approach, known as flux-difference splitting (FDS), has the desirable property of accurately resolving shock waves as well as contact discontinuities. Although some Riemann solvers, such as Roe's approximate Riemann solver [20], admit rarefaction shocks that do not satisfy the entropy condition, this flaw can be easily handled by simple entropy fix

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procedures [9,11] in one-dimensional case. However, when extending the flux-difference schemes to several spatial dimensions by so-called grid-aligned finite-volume approach or dimensional splitting method, they can on occasions fail quite spectacularly. A description of a number of failings of exact and approximate Riemann solvers for the Euler equations of gasdynamics, especially the “odd–even decoupling” and the “carbuncle” phenomena, can be found in Quirk’s paper [19].

In order to construct robust shock-capturing schemes, some correction routines [15,18,19,23] to the FDS schemes have been proposed to cure the multidimensional shock instabilities [15] that are often manifested by the odd–even decoupling and the carbuncle phenomenon [19]. All these corrections involve the detection for cell faces deemed as susceptible to the shock instabilities. At these faces, the original numerical flux functions are either modified with some special entropy fix procedures resulting from multidimensional considerations, or, replaced by more dissipative flux functions. These remedies have been proved to be useful, but may fail when the underlying problem involves interactions of complex flow features. It is interesting to note that, in [15], the shock instabilities can be avoided by a proper design of mass flux. This suggests that appropriate designing of numerical fluxes may eliminate the shock instabilities without relying on specific detection techniques.

The catastrophic carbuncle instability for FDS schemes is a particular problem for multidimensional computation. Therefore, in the construction of numerical fluxes, it is helpful to take the multidimensional effects into consideration. Levy et al. [14] categorized the upwind numerical methods for multidimensional computation into four types, namely, grid-aligned methods, rotation methods, rotation/interpolation methods and truly (genuine) multidimensional convection schemes. The genuine multidimensional schemes [1,2,4,6,13] are very attractive because they model the multidimensional wave propagation as faithfully as possible. However, these schemes are usually quite complex and computationally expensive. Even the rotation/interpolation approach proposed in [14] turns out to be very expensive because the left and right cell face states associated with each upwind direction need to be computed with a rather complicated interpolation procedure. On the other hand, the rotated methods using the same set of face data in every upwind direction are more efficient than their rotation/interpolation counterparts, which is especially true for non-Cartesian meshes. Furthermore, this type of methods can be easily extended to higher order of accuracy through the formal use of MUSCL interpolations [27] or ENO reconstructions [8]. Therefore, we focus on the design of FDS schemes that are free from shock instability based on rotated Riemann solvers and MUSCL interpolations in this paper. It should be noted that the use of rotated Riemann solvers in the present paper is to improve the robustness of the FDS schemes rather than to capture shocks and shear waves with higher resolution. Therefore, the numerical method proposed in this paper is not necessarily more accurate than its grid-aligned counterpart.

In Section 2, the rotation method is reformulated and generalized based on the geometrical considerations and the rotational invariance property of gasdynamic Euler equations. This approach is called generalized rotation methods in this paper. In Section 3, we present the rotated form of Roe’s approximate Riemann solver, and the effect of upwinding directions is discussed. It is found that if the vector of the velocity-difference at a cell face is chosen as the direction of upwinding, the resulted scheme is shock instability free without explicitly detecting the cell faces that are susceptible to the shock instability. Moreover, the dissipation property of the rotated
Roe’s Riemann solver is discussed in this section. Numerical results are presented in Section 4 followed by a summary in Section 5.

2. The generalized rotated flux function

2.1. The finite-volume scheme

We consider the two-dimensional Euler equations describing the flows of inviscid fluids. In conservation form the equations are

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0,$$

where the conserved variables are $U = [\rho, \rho u, \rho v, \rho E]^T$ and the inviscid flux vectors are

$$F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u H \end{bmatrix}, \quad G = \begin{bmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ \rho v H \end{bmatrix}.$$  

$H = E + p/\rho$ is the enthalpy. This set of equations are closed by the equation-of-state of ideal gas

$$p = (\gamma - 1)\rho \left[ E - \frac{u^2 + v^2}{2} \right].$$

We consider some two-dimensional domain in $x$–$y$ space and assume it is discretized into structured quadrilateral control volumes. Examples of typical control cells are shown in Fig. 1. Finite-volume schemes for Eq. (1) are obtained by considering the control volume balance equation
where $\Omega_{i,j}$ is a control volume, $\partial \Omega_{i,j}$ is the boundary of $\Omega_{i,j}$, $\mathbf{H} = \mathbf{F} + \mathbf{G}$ is the tensor of the fluxes, $\mathbf{n} = n_i \mathbf{i} + n_j \mathbf{j}$ is the outward unit vector normal to the surface $\partial \Omega_{i,j}$. For a quadrilateral control volume with its faces denoted by $I_k$ ($k = 1, \ldots, 4$), the flux through the control volume boundary $\partial \Omega_{i,j}$ can be written as

$$
\int_{\partial \Omega_{i,j}} \mathbf{H} \cdot \mathbf{n} d\mathbf{l} = \sum_{k=1}^{4} \int_{I_k} \mathbf{H} \cdot \mathbf{n} d\mathbf{l}.
$$

We introduce the average of $\mathbf{U}$ inside $\Omega_{i,j}$ by

$$
\mathbf{U}_{i,j} = \frac{\int_{\Omega_{i,j}} \mathbf{U} d\mathbf{x} d\mathbf{y}}{\int_{\Omega_{i,j}} d\mathbf{x} d\mathbf{y}}.
$$

Substituting Eqs. (3) and (4) into (2) gives

$$
\frac{\partial \mathbf{U}_{i,j}}{\partial t} = - \frac{1}{|\Omega_{i,j}|} \sum_{k=1}^{4} \int_{I_k} \mathbf{H} \cdot \mathbf{n} d\mathbf{l},
$$

where $|\Omega_{i,j}| = \int_{\Omega_{i,j}} d\mathbf{x} d\mathbf{y}$ is the volume of $\Omega_{i,j}$. In this paper, we are interested in the finite-volume scheme that is at most spatially second order accurate. Therefore, it is sufficient to integrate the flux terms in Eq. (5) by using the midpoint rule. Eq. (5) is now approximated as

$$
\frac{\partial \mathbf{U}_{i,j}}{\partial t} = - \frac{1}{|\Omega_{i,j}|} \sum_{k=1}^{4} \mathbf{H}_k \cdot \mathbf{n}_k \Delta l_k,
$$

where $\mathbf{n}_k$ is the outward unit vector normal to face $I_k$, $\Delta l_k$ is the length of $I_k$ and $\mathbf{H}_k$ is the tensor of fluxes at the midpoint of $I_k$. Eq. (6) is a semi-discrete finite-volume scheme. Assuming that we have chosen a time integration scheme, the only open question is how to evaluate the flux components normal to cell boundary, namely $\mathbf{H}_k \cdot \mathbf{n}_k$ ($k = 1, 2, 3, 4$).

According to Levy et al. [14], there are four types of methods to compute $\mathbf{H}_k \cdot \mathbf{n}_k$ ($k = 1, 2, 3, 4$), including the grid-aligned method and the rotation method. In the following subsections, we will review the construction of grid-aligned flux function and present the construction of generalized rotated flux function that can be considered as the reformulation and generalization of the rotation method.

2.2. The grid-aligned flux function

Following [26], we introduce the rotational invariant property of Euler equations. For the two-dimensional case, we have

$$
\mathbf{H}_k \cdot \mathbf{n}_k = \mathbf{F}_k n_{xk} + \mathbf{G}_k n_{yk} = \mathbf{T}_k^{-1} \mathbf{F}(\mathbf{T}_k \mathbf{U}_k) \quad (k = 1, 2, 3, 4),
$$

where $n_{xk}$ and $n_{yk}$ are the $x$- and $y$-components of $\mathbf{n}_k$ respectively, $\mathbf{T}_k$ is the rotation matrix and $\mathbf{T}_k^{-1}$ is its inverse, namely
We denote \( \mathbf{U}_k \equiv \mathbf{T}_k \mathbf{U}_k \), which is the vector of conserved variables that is aligned with \( \hat{x} \) in the rotated Cartesian frame \((\hat{x}, \hat{y})\) as shown in Fig. 2. It follows from Eq. (7) that the semi-discrete finite-volume scheme (6) becomes
\[
\frac{\partial \mathbf{U}_{i,j}}{\partial t} = - \frac{1}{|\Omega_{i,j}|} \sum_{k=1}^{4} \mathbf{T}_k^{-1} \mathbf{F}(\hat{\mathbf{U}}_k) \Delta l_k.
\]

The key idea of the grid-aligned method is to compute the flux function \( \mathbf{F}(\hat{\mathbf{U}}_k) \) in terms of the augmented one-dimensional system [26]
\[
(\hat{\mathbf{U}}_k)_t + (\hat{\mathbf{F}}_k)_{\hat{x}} = 0,
\]
where \( \hat{\mathbf{F}} = \mathbf{F}(\hat{\mathbf{U}}) \). This approach is quite general and any flux formulation for one-dimensional problem can be extended into a multidimensional flux function. For FDS schemes, \( \mathbf{F}(\hat{\mathbf{U}}_k) \) can be evaluated by (approximately) solving the Riemann problem associated with Eq. (8):
\[
\begin{aligned}
(\hat{\mathbf{U}}_k)_t + (\hat{\mathbf{F}}_k)_{\hat{x}} &= 0, \\
\hat{\mathbf{U}}_k(\hat{x}, 0) &= \begin{cases} \\
\hat{\mathbf{U}}_k^L & \text{if } \hat{x} < 0, \\
\hat{\mathbf{U}}_k^R & \text{if } \hat{x} > 0.
\end{cases}
\end{aligned}
\]

2.3. The generalized rotated flux function

The shortcomings of the grid-aligned method have been well recognized [12,16,21] and many efforts have been directed to design multidimensional schemes. In this paper, we account for the multidimensional effects by decomposing \( \mathbf{n}_k \), the outward unit vector normal to face \( I_k \) in Eq. (6), into the summation of two or more vectors, namely
\( \mathbf{n}_k = \sum_{m=1}^{N} \mathbf{\hat{n}}_k^m (N \geq 2), \)

or equivalently

\( \mathbf{n}_k = \sum_{m=1}^{N} \alpha_k^m \mathbf{n}_k^m (N \geq 2), \) (9)

where \( \mathbf{n}_k^m \) is the unit vector in the direction of \( \mathbf{\hat{n}}_k^m. \) The use of Eq. (9) and the rotational invariant property of Euler equations lead to

\[
\mathbf{H}_k \cdot \mathbf{n}_k = \sum_{m=1}^{N} \alpha_k^m (\mathbf{F}_k h_k^m + \mathbf{G}_k n_k^m) = \sum_{m=1}^{N} \alpha_k^m (\mathbf{T}_k^m)^{-1} \mathbf{F}(\mathbf{T}_k^m \mathbf{U}_k) \quad (k = 1, 2, 3, 4),
\]

where \( \mathbf{T}_k^m \) is the rotation matrix corresponding to \( \mathbf{n}_k^m. \) Eq. (6) can now be written as

\[
\frac{\partial \mathbf{U}_{ij}}{\partial t} = -\frac{1}{|\Omega_{ij}|} \sum_{k=1}^{4} \sum_{m=1}^{N} (\mathbf{T}_k^m)^{-1} \hat{\mathbf{F}}_k^m \alpha_k^m \Delta I_k,
\]

where \( \hat{\mathbf{F}}_k^m = \mathbf{F}(\hat{\mathbf{U}}_k^m), \hat{\mathbf{U}}_k^m = \mathbf{T}_k^m \mathbf{U}_k. \) As in the grid-aligned method, the flux \( \hat{\mathbf{F}}_k^m \) is evaluated in terms of the augmented one-dimensional system

\[
(\hat{\mathbf{U}}_k^m)_t + (\hat{\mathbf{F}}_k^m)_{x_m} = 0,
\]

where \( \hat{x}_m \) is aligned with \( \mathbf{n}_k^m. \) In this approach, \( \mathbf{H}_k \cdot \mathbf{n}_k \) \((k = 1, 2, 3, 4),\) the flux components normal to cell boundary \( I_k, \) are computed according to

\[
\mathbf{H}_k \cdot \mathbf{n}_k = \sum_{m=1}^{N} \alpha_k^m (\mathbf{T}_k^m)^{-1} \hat{\mathbf{F}}_k^m \quad (k = 1, 2, 3, 4),
\]

which involves the evaluation of fluxes in \( N \) directions with procedures similar to the grid-aligned method. If we restrict that

\[
\begin{align*}
N &= 2, \\
\mathbf{n}_k^1 \cdot \mathbf{n}_k^2 &= 0.
\end{align*}
\]

Eq. (11) is reduced to the rotated flux function [14]. Therefore, we call Eq. (11) the generalized rotated flux function.

The purpose for the introduction of the generalized rotated flux function in this paper is to facilitate the derivations and discussions in the next section, but we believe this flux formulation can also serve as a building block for developing new numerical schemes. The decomposition of \( \mathbf{n}_k \) into \( N \) vectors is purely a geometrical procedure, but physical features of the flow problem can be taken into account to determine how to make the decomposition. Furthermore, it is not necessary to compute all fluxes \( \hat{\mathbf{F}}_k^m \) \((m = 1, \ldots, N)\) with the same scheme. We can, for example, calculate \( \hat{\mathbf{F}}_k^1 \) with FDS methods and calculate \( \hat{\mathbf{F}}_k^2 \) with flux-vector splitting (FVS) [25,28] schemes or even central differencing. Of course, the choice of flux formulations should also be based on, or at least partly based on, consideration of the flow physics. The flexibility to make the decomposition in Eq. (9) and to select the flux functions in each direction makes it possible to obtain optimized
numerical schemes for solving hyperbolic conservation laws. However, this optimization of the generalized rotated flux function will not be pursued in this paper. We will focus on the rotated method and assume that Eq. (12) always holds in the rest parts of this paper. Additionally, both $F^1_k$ and $F^2_k$ will be computed by the FDS scheme based on Roe’s approximate Riemann solver.

3. The rotated Roe scheme

3.1. The rotated flux function based on Roe’s approximate Riemann solver

In deriving the rotated flux function, it is convenient to write Eq. (9) in the following form (with $N = 2$):

$$
\mathbf{n}_k = \sum_{m=1}^{2} |\mathbf{z}_k^m| \hat{\mathbf{n}}_k^m.
$$

$\hat{\mathbf{n}}_k^m \equiv \text{sign}(\mathbf{z}_k^m)\mathbf{n}_k^m$ is called the normalized unit vector corresponding to $\mathbf{n}_k^m$. For brevity, we consider face $i_{i+1/2,j}$ only. When using Roe’s approximate Riemann solver to calculate $F^m_{i+1/2,j}$ ($m = 1, 2$), the flux $\Phi \equiv H \cdot \mathbf{n}$ in Eq. (11) can be written as

$$
\Phi_{i+1/2,j} = \frac{1}{2} (\Phi^L_{i+1/2,j} + \Phi^R_{i+1/2,j}) - \frac{1}{2} \left[ \sum_{m=1}^{2} |\mathbf{z}_{i+1/2,j}^m| \sum_{l=1}^{4} \left( \mathbf{\tilde{\Omega}}_l^m \mathbf{\tilde{F}}_l^m \right)_{i+1/2,j} \right],
$$

(13)

where $\Phi^L_{i+1/2,j} = \Phi(\mathbf{U}^L_{i+1/2,j})$, $\Phi^R_{i+1/2} = \Phi(\mathbf{U}^R_{i+1/2,j})$, $\mathbf{U}^L_{i+1/2,j}$ and $\mathbf{U}^R_{i+1/2,j}$ are left and right states of the conservative variables at face $i_{i+1/2,j}$. For a spatially first order scheme, the left and right states are taken to be the average quantities in the cells on either side of the cell face

$$
\mathbf{U}^L_{i+1/2,j} = \underline{\mathbf{U}}_{i,j}, \quad \mathbf{U}^R_{i+1/2,j} = \underline{\mathbf{U}}_{i+1,j}.
$$

We denote the Roe-averaged values by tildes throughout this paper and define the velocity components parallel and normal to $\mathbf{n}_{i+1/2,j}$ respectively by

$$
g_m = u \hat{n}_x^m + v \hat{n}_y^m,
$$

$$
r_m = -u \hat{n}_y^m + v \hat{n}_x^m.
$$

Using these notations, the other terms in Eq. (13) can be explained as follows. $\mathbf{\tilde{R}}_l^m$ ($l = 1, 2, 3, 4$) is the $l$th eigenvector of matrix $\mathbf{\tilde{C}}_{i+1/2,j}^m = \frac{\partial(H \cdot \mathbf{n}^m)}{\partial \mathbf{U}_{i+1/2,j}}$, namely

$$
\mathbf{\tilde{R}}_1^m = [1, \hat{u} + \tilde{a} \hat{n}_x, \hat{v} + \tilde{a} \hat{n}_y, \hat{H} + \tilde{a} \tilde{q}_m]^T,
$$

$$
\mathbf{\tilde{R}}_2^m = [1, \hat{u} - \tilde{a} \hat{n}_x, \hat{v} - \tilde{a} \hat{n}_y, \hat{H} - \tilde{a} \tilde{q}_m]^T,
$$

$$
\mathbf{\tilde{R}}_3^m = [0, -\tilde{a} \hat{n}_y, \tilde{a} \hat{n}_x, \tilde{a} \tilde{r}_m]^T,
$$

$$
\mathbf{\tilde{R}}_4^m = [1, \tilde{u}, \tilde{v}, (\tilde{u}^2 + \tilde{v}^2)]^T.
$$
where \( a = \sqrt{\gamma p/\rho} \) is the speed of sound. \( \tilde{\Omega}^m \), for \( l = 1,2,3,4 \), are respectively the strength of +acoustic, −acoustic, shear and entropy waves in the direction parallel to \( \mathbf{n}_{i+1/2,j}^m \), which can be written as components of vector \( \tilde{\Omega}^m \)

\[
\tilde{\Omega}^m = \begin{bmatrix}
\frac{1}{\alpha^2} (\Delta p + \tilde{\rho} \tilde{a} \Delta q_m) \\
\frac{1}{\alpha^2} (\Delta p - \tilde{\rho} \tilde{a} \Delta q_m) \\
\frac{1}{\alpha^2} \tilde{\rho} \Delta r_m \\
\frac{1}{\alpha^2} (\tilde{a}^2 \Delta p - \Delta p)
\end{bmatrix},
\]

where \( \Delta(\cdot) = (\cdot)^R - (\cdot)^L \). \( \tilde{\lambda}_l^m \) \( (l = 1,2,3,4) \) are the eigenvalues of \( \tilde{C}_{i+1/2,j}^m \), namely

\[
\tilde{\lambda}_1^m = \tilde{q}_m + \tilde{a},
\]
\[
\tilde{\lambda}_2^m = \tilde{q}_m - \tilde{a},
\]
\[
\tilde{\lambda}_3^m = \tilde{\lambda}_4^m = \tilde{q}_m.
\]

The fluxes at faces other than \( I_{i+1/2,j} \) can be written in forms similar to Eq. (13).

3.2. Choice of \( \mathbf{n}_k^m \) \( (m = 1,2) \)

In order to calculate the fluxes with rotated flux function, \( \mathbf{n}_k^m \) \( (m = 1,2) \) must be determined first. Since \( \mathbf{n}_k^1 \cdot \mathbf{n}_k^2 = 0 \), we can assume \( \mathbf{n}_k^2 = \mathbf{k} \times \mathbf{n}_k^1 \), where \( \mathbf{k} = \mathbf{i} \times \mathbf{j} \). Let

\[
\mathbf{n}_k = \sum_{m=1}^{2} \chi_k^m \mathbf{n}_k^m.
\]

(14)

It is easily seen that

\[
\chi_k^1 = \mathbf{n}_k \cdot \mathbf{n}_k^1,
\]
\[
\chi_k^2 = \mathbf{n}_k \cdot \mathbf{n}_k^2.
\]

Therefore, all we need is to determine \( \mathbf{n}_k^1 \). Unlike in [14], it is not necessary to distinguish between dominant upwind direction and minor upwind direction because we use exactly the same Riemann solver in both directions. Also in [14], it is proposed that \( \mathbf{n}_k^1 \) can be chosen as the flow direction, pressure-gradient direction, or velocity-magnitude-gradient direction. Numerical tests to be presented in Section 4 indicate that none of these methods can remove the shock instability completely. Therefore, other physically meaningful methods are needed to determine the upwind direction.

In the present work, we propose to align \( \mathbf{n}_k^1 \) with the velocity-difference vector \( \Delta \mathbf{u} = \Delta u \mathbf{i} + \Delta v \mathbf{j} \), which has been used in [3,22] to determine the upwind direction in some different methods. In practice, at interface \( I_{i+1/2,j} \), \( \mathbf{n}_{i+1/2,j}^1 \) is determined by
than decomposition Eq. (14) and set section in terms of numerical dissipations of the schemes and in Section 4 by a test case.

We point out that the use of the velocity-difference as the upwind direction can effectively eliminate the shock instabilities. The effects of upwind directions will be discussed in next subsection in terms of numerical dissipations of the schemes and in Section 4 by a test case.

The rotated flux function can be easily extended to three-dimensional cases. We still use the decomposition Eq. (14) and set $n^1_k$ to align with the direction of velocity-difference vector. Now $n^2_k$ can be chosen as

$$n^2_k = (n^1_k \times n^1_k) \times n^1_k.$$ 

Again the parameters $z^1_k$ and $z^2_k$ are calculated by using Eq. (15).

### 3.3. The dissipation properties of the rotated Roe scheme

The dissipation properties of the FDS schemes are in close relation to the shock instability phenomena. On Cartesian meshes, the truncation error equations for the semi-discrete first order finite-volume scheme employing grid-aligned flux function of Roe take the following form [23]:

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = \frac{1}{2} \Delta x \frac{\partial}{\partial x} \left( |A(U)| \frac{\partial U}{\partial x} \right) + \frac{1}{2} \Delta y \frac{\partial}{\partial y} \left( |B(U)| \frac{\partial U}{\partial y} \right),$$

where $A = \partial F/\partial U$, $B = \partial G/\partial U$. Therefore, the dissipation property of the grid-aligned method can be characterized by the eigenvalues of $|A|$ and $|B|$. If there is a normal shock wave well aligned with $x$-axis and the flow field is subjected to small numerical disturbances, the shock instabilities may take place at locations near or inside the shock layer where $|A|$ is multiplicity 2 singular. It is thus believed that the presence of the shock wave and the vanishing of eigenvalues corresponding to the contact and shear waves in the direction parallel to the shock front will initiate a rather rapid amplification of the disturbances and lead to instability eventually. Xu and Li [31] explained how this instability was formed in terms of the aerodynamic theory after giving a full analysis about the dissipation properties of FDS (and FVS) schemes. It is also useful to analyze the dissipation properties for rotated flux function. Here we only examine the dissipations corresponding to the contact and shear waves because they are not only closely related to the shock instability or carbuncle phenomenon but also have great influence on capturing contact and shear wave, which is considered to be important for viscous computation. To compare the linear wave dissipations between the rotated FDS method and the grid-aligned FDS method, we note that the grid-aligned flux function can be considered as a special case of the rotated flux function. If $n^1_k = n_k$, we have

$$n^1_{i+1/2,j} = \begin{cases} n_{i+1/2,j} & \text{if } \sqrt{(\Delta u_{i+1/2,j})^2 + (\Delta v_{i+1/2,j})^2} \leq \varepsilon, \\ \frac{\Delta u_{i+1/2,j} \hat{i} + \Delta v_{i+1/2,j} \hat{j}}{\sqrt{(\Delta u_{i+1/2,j})^2 + (\Delta v_{i+1/2,j})^2}} & \text{otherwise}, \end{cases}$$

where $\varepsilon$ is a small positive number. According to Eq. (16), when the velocity-difference is larger than $\varepsilon$, the velocity-difference vector is used to determine $n^1_{i+1/2,j}$; otherwise, the rotated Riemann solver is reduced to grid-aligned one in order to avoid the noise. The use of the velocity-difference vector as an upwind direction is of physical significance. If there is a shock or a shear wave at the cell interface, the shock will propagate in the direction of $n^1_k$ and the shear wave will move in the direction of $n^2_k$ [22].
\( x_1^1 = 1, x_2^2 = 0 \) and the rotated flux function will be reduced to the corresponding grid-aligned flux function.

Taking cell face \( I_{i+1/2,j} \) as an example, the dissipation term corresponding to the entropy wave for the rotated Roe flux is

\[
(D_4^R)_{i+1/2,j} \equiv \frac{1}{2} \sum_{m=1}^{2} \left( |x_i^{m} I_{i+1/2,j} \tilde{\lambda}_4^m | \bar{\Omega}_4^m \tilde{\bar{R}}_4^m \right)_{i+1/2,j} = \frac{1}{2} |(\tilde{\lambda}_4^R)_{i+1/2,j}| |(\bar{\Omega}_4 \tilde{\bar{R}}_4)_{i+1/2,j}|, \tag{17}
\]

where \( \bar{\Omega}_4 = \tilde{\Omega}_4^1 = \tilde{\Omega}_4^2, \bar{R}_4 = \tilde{\bar{R}}_4^1 = \tilde{\bar{R}}_4^2 \) and \( |(\tilde{\lambda}_4^R)_{i+1/2,j}| = \sum_{m=1}^{2} |x_i^{m} I_{i+1/2,j} \tilde{\lambda}_4^m|_{i+1/2,j} \). For the grid-aligned flux function, the dissipation term corresponding to the entropy wave is given by

\[
(D_4^G)_{i+1/2,j} = \frac{1}{2} |(\tilde{\lambda}_4)_{i+1/2,j}| |(\bar{\Omega}_4 \tilde{\bar{R}}_4)_{i+1/2,j}|, \tag{18}
\]

where \( \tilde{\lambda}_4 = \tilde{\lambda}_4^1 = \tilde{\lambda}_4^2, \tilde{\bar{R}}_4 = \tilde{\bar{R}}_4^1 = \tilde{\bar{R}}_4^2 \). According to Eqs. (17) and (18), the numerical dissipations for the rotated and grid-aligned entropy wave can be measured by the wave speeds \(|(\tilde{\lambda}_4^R)_{i+1/2,j}| \) and \(|(\tilde{\lambda}_4)_{i+1/2,j}| \) respectively. It can be verified that

\[
|(\tilde{\lambda}_4^R)_{i+1/2,j}| = |x_i^{1} I_{i+1/2,j} (\tilde{\lambda}_4^1)_{i+1/2,j}| + |x_i^{2} I_{i+1/2,j} (\tilde{\lambda}_4^2)_{i+1/2,j}| \geq |(\tilde{\lambda}_4)_{i+1/2,j}|.
\]

This implies, for the entropy wave, the rotated flux function is always more dissipative than the grid-aligned flux function. Furthermore, if

\[
(\tilde{\lambda}_4)_{i+1/2,j} (\tilde{\lambda}_4^1)_{i+1/2,j} \geq 0 \text{ and } (\tilde{\lambda}_4)_{i+1/2,j} (\tilde{\lambda}_4^2)_{i+1/2,j} \geq 0, \tag{19}
\]

then it can be shown that

\[
|(\tilde{\lambda}_4^R)_{i+1/2,j}| = |(\tilde{\lambda}_4)_{i+1/2,j}|,
\]

i.e., the entropy wave dissipation for the rotated flux function is the same as that for grid-aligned flux function. Eq. (19) is equivalent to that the velocity vector on the cell interface lies between \( \mathbf{n}_i^{1} I_{i+1/2,j} \) and \( \mathbf{n}_i^{2} I_{i+1/2,j} \) (or \( -\mathbf{n}_i^{1} I_{i+1/2,j} \) and \( -\mathbf{n}_i^{2} I_{i+1/2,j} \)), which is shown by the shaded region in Fig. 3a.

The dissipation term corresponding to shear wave is

\[
(D_3^R)_{i+1/2,j} \equiv \frac{1}{2} \sum_{m=1}^{2} \left( |x_i^{m} I_{i+1/2,j} | \bar{\Omega}_3^m \tilde{\bar{R}}_3^m \right)_{i+1/2,j},
\]

When \( \mathbf{n}_i^{1} I_{i+1/2,j} = [\Delta u_i^{1}, \Delta v_i^{1}] \sqrt{\left(\Delta u_i^{1/2,j}\right)^2 + \left(\Delta v_i^{1/2,j}\right)^2} \) is used to determine the upwind direction, we have \( \bar{\Omega}_3^1 = 0 \) and

\[
(D_3^R)_{i+1/2,j} = -\frac{1}{2} \bar{\rho}_{i+1/2,j} \sqrt{\left(\Delta u_i^{1/2,j}\right)^2 + \left(\Delta v_i^{1/2,j}\right)^2} |(\bar{q}_2)_{i+1/2,j}| |x_i^{2} I_{i+1/2,j}| \begin{bmatrix} 0 \\ -\bar{n}_y^2 \\ -\bar{n}_z^2 \\ \bar{r}_2 \end{bmatrix}_{i+1/2,j}.
\]
Fig. 3. Comparisons of the linear wave dissipations between the rotated Roe scheme and the grid-aligned Roe scheme. On the cell face $I_{i+1/2,j}$, the linear wave dissipations are affected by the relative directions among the interface velocity vector, $\mathbf{n}_{i+1/2,j}$ and $\mathbf{n}_{i+1/2,j}$ ($\mathbf{n}_{i+1/2,j}$). The shaded regions show the ranges of interface velocity directions. $A1$ and $A2$ are the angles between the corresponding lines. (a) In the shaded region, the dissipation term associated with the entropy wave for the rotated FDS scheme is the same as that for the grid-aligned FDS scheme. (b) In the shaded region, the numerical shear stress for the rotated FDS scheme is smaller than that for the grid-aligned FDS scheme. (c) In the shaded region, the energy flux dissipation associated with the shear wave for the rotated FDS scheme is smaller than that for the grid-aligned FDS scheme. (d) The shaded region is the intersection of the shaded regions in (a), (b) and (c). (e) The shaded region is the intersection of the un-shaded regions in (a), (b) and (c).
For the grid-aligned flux function, the shear wave dissipation term can be written as

\[
(D^G_{3})_{i+1/2,j} = -\frac{1}{2} \bar{\rho}_{i+1/2,j} \sqrt{(\Delta u_{i+1/2,j})^2 + (\Delta v_{i+1/2,j})^2} |(\vec{q})_{i+1/2,j}| a_{i+1/2,j}^2 \begin{bmatrix} 0 \\ -n_y \\ n_x \end{bmatrix} \text{.}
\]

Since the eigenvectors corresponding to shear wave for rotated and grid-aligned flux functions are different, we examine the numerical dissipation by considering the momentum equation and the energy equation separately. The magnitude of numerical dissipation for the rotated and grid-aligned methods can be obtained respectively by

\[
(S^R)_{i+1/2,j} = \frac{1}{2} \bar{\rho}_{i+1/2,j} \sqrt{(\Delta u_{i+1/2,j})^2 + (\Delta v_{i+1/2,j})^2} |x_{i+1/2,j}(\vec{q})_{i+1/2,j}|^2
\]

and

\[
(S^G)_{i+1/2,j} = \frac{1}{2} \bar{\rho}_{i+1/2,j} \sqrt{(\Delta u_{i+1/2,j})^2 + (\Delta v_{i+1/2,j})^2} |x_{i+1/2,j}(\vec{q})_{i+1/2,j}|^2.
\]

Therefore, in terms of shear stress, the rotated flux function may be more or less dissipative than the grid-aligned flux function. If

\[
|\vec{q}_{i+1/2,j}| \geq |(\vec{q})_{i+1/2,j}|,
\]

or the velocity vector on the cell interface lies in the shaded region in Fig. 3b, the rotated flux function is less dissipative than the grid-aligned flux function. For energy flux corresponding to shear wave, it is easy to verify that if

\[
|\vec{q}_{i+1/2,j} \cdot \vec{r}_{i+1/2,j}| \geq |(\vec{q})_{i+1/2,j} \cdot (\vec{r})_{i+1/2,j}|,
\]

the grid-aligned flux function is more dissipative than the rotated flux function, which corresponds to the fact that the velocity vector on the cell interface lies in the shaded region in Fig. 3c.

In Fig. 3d, the shaded region (Region R1) is the intersection of the shaded regions in Fig. 3a–c. In this region, the linear wave dissipation for the rotated flux function is smaller than that for the grid-aligned flux function. An example for such case is a pure shear wave with velocity vectors that are not aligned with grid lines, for which \( \vec{u}_{i+1/2,j} + \vec{v}_{i+1/2,j} \) is parallel to \( \Delta u_{i+1/2,j} + \Delta v_{i+1/2,j} \) and therefore lies in Region R1. The shaded region (Region R2) in Fig. 3e is the intersection of the un-shaded regions in Fig. 3a–c. If the velocity vector at the cell interface falls into this region, then the linear wave dissipation for rotated flux function is larger than that for grid-aligned flux function.

It should be noted that if a shear wave or a shock wave is well aligned with the grid line, or if \( n_{i+1/2,j} \) is almost parallel or normal to \( n_{i+1/2,j} \), the rotated flux function will essentially reduce to the grid-aligned flux function. As a result, for viscous computation on structured body-fitted meshes, the rotated FDS schemes can be as accurate as the grid-aligned method in capturing the near grid-aligned boundary layers and shear layers.

Next, we will analyze the behavior of rotated flux function in terms of the linear wave dissipation at place where the shock instability might occur. We consider, in a two-dimensional domain, two rectangular control volumes \((i, j)\) and \((i + 1, j)\) as shown in Fig. 4. Uniform conditions in \( x \)-direction are assumed, with \( u_{i,j} = u_{i+1,j} = 0, \ v_{i,j} = v_{i+1,j} = v_0, \ p_{i,j} = p_{i+1,j} = p_0 \) and \( \rho_{i,j} = \rho_{i+1,j} = \rho_0 \). On the interface between these two control volumes, \( I_{i+1/2,j} \), we have

\[
\begin{align*}
\bar{\rho}_{i+1/2,j} &= \frac{\rho_{i,j} \rho_{i+1,j}}{\rho_{i+1/2,j}^2} \bar{\rho}_{i,j} + \frac{\rho_{i+1,j} \rho_{i+1,j}}{\rho_{i+1/2,j}^2} \bar{\rho}_{i+1,j} = \frac{\rho_{i,j} \rho_{i+1,j}}{\rho_{i+1/2,j}^2} \bar{\rho}_{i,j} + \frac{\rho_{i+1,j} \rho_{i+1,j}}{\rho_{i+1/2,j}^2} \bar{\rho}_{i+1,j} \approx \frac{\rho_{i,j} \rho_{i+1,j}}{\rho_{i+1/2,j}^2} \bar{\rho}_{i,j} \approx \frac{\rho_{i+1,j} \rho_{i+1,j}}{\rho_{i+1/2,j}^2} \bar{\rho}_{i+1,j},
\end{align*}
\]
This means that the rotated flux function and the grid-aligned flux function behave identically the same without any numerical dissipation for the linearly degenerated field (and also for genuinely non-linear fields) if the flow field is uniform. We assume that there is a horizontal shock wave and cell \((i, j)\) and cell \((i + 1, j)\) are adjacent to or inside the numerical shock layer. When the flow field is perturbed due to numerical oscillations and/or grid distortions, the grid-aligned FDS schemes will often lead to catastrophic failings. It is believed that it is a transverse numerical instability associated with the shock wave due to the lack of numerical dissipations for linear field on the vertical face of the control volumes (e.g. face \(I_{i+1/2,j}\)) [15]. We denote the perturbed flow quantities with \(\phi^* = \phi_0 + \phi'\) (\(\phi = u, v, p, \rho\)) and categorize the disturbances into two types. In the first type, the disturbances are very small or grid-aligned in nature, which can be represented by

\[
\sqrt{(\Delta u_{i+1/2,j})^2 + (\Delta v_{i+1/2,j})^2} \leq \varepsilon
\]

or

\[
|\Delta u_{i+1/2,j}| \ll |\Delta v_{i+1/2,j}|
\]

or

\[
|\Delta u_{i+1/2,j}| \gg |\Delta v_{i+1/2,j}|.
\]

In this case, the rotated method will essentially reduce to the grid-aligned method. In the second type, the disturbances are multidimensional i.e., \(|\Delta u_{i+1/2,j}|\) and \(|\Delta v_{i+1/2,j}|\) are in the same order with

\[
\sqrt{(\Delta u_{i+1/2,j})^2 + (\Delta v_{i+1/2,j})^2} > \varepsilon.
\]

In this case, if \(|u'| \ll |v_0|\) and \(|v'| \ll |v_0|\) are assumed, we have

\[
u_{i+1/2,j} = \tilde{v}_{i+1/2,j} = v_0 j.
\]

Referring to Fig. 3e, \(\bar{u}_{i+1/2,j} + \tilde{v}_{i+1/2,j}\) always falls in to Region R2 (in this case, \(n_{i+1/2,j} = i\)). Therefore, when the disturbances are multidimensional, the use of the rotated flux function effectively increases the numerical dissipations for linear field. Numerical tests indicate that the shock instabilities can be eliminated completely. By distinguishing these two types of disturbances, we can also conclude that the multidimensional disturbances are responsible to the shock instability. It is interesting to note that according to Xu and Li’s explanation [31] on the
shock instability, when the shock instability happens in the subsonic region, the converging (diverging) streamline will become more converging (diverging). This indicates the numerical perturbations will be multidimensional in nature when the instability is formed.

If \( \mathbf{n}^{1}_{i+1/2,j} \) is chosen as the flow direction, we have \( \mathbf{n}^{1}_{i+1/2,j} \approx \mathbf{0} \), \( \mathbf{n}^{2}_{i+1/2,j} \approx \mathbf{i} \) and the rotated flux function is almost identical to the grid-aligned flux function. As a result, the disturbances cannot be dissipated effectively to avoid the instability. If \( \mathbf{n}^{1}_{i+1/2,j} \) is determined by pressure-gradient or velocity-magnitude-gradient, the rotated flux function becomes also near grid-aligned when the control volumes under consideration are adjacent to or inside the numerical shock layer. However, when the control volumes are in the uniform flow region and the gradient computation is not affected by the presence of the shock wave, the use of the gradient of certain flow quantity as the upwind direction will make similar effects to the use of the velocity-difference. We therefore expect, when the upwind direction is determined by the gradient of some flow quantity, the shock instability cannot be removed completely but can be restricted in regions inside or adjacent to the numerical shock layer if the flow is almost uniform near shock.

### 3.4. Extension to higher order accuracy

Any method having higher order accuracy in space or time for the grid-aligned method can be applied to the rotated method. For completeness, the methods used to compute the test cases in Section 4 are presented here.

Second order spatial accuracy can be achieved by the MUSCL approach of Van Leer [27]. It is well known that the reconstruction may be carried out in local characteristic variables to avoid oscillations [10]. However, when the rotated flux function is used, it is not clear if the grid-aligned characteristics should be used by considering the increase of computational time and programming complexity. We therefore use the component-wise reconstruction in terms of the conservative variables. At interface \( I_{i+1/2,j} \), the \( \mathbf{U}^L \) and \( \mathbf{U}^R \) are computed with

\[
\begin{align*}
\mathbf{U}^L_{i+1/2,j} &= \mathbf{U}_{i,j} + \frac{s_{i,j}^L}{4} \left[ \left( 1 + \frac{s_{i,j}^L}{3} \right) A_{i,j}^i + \left( 1 - \frac{s_{i,j}^L}{3} \right) \nabla_{i,j} \right], \\
\mathbf{U}^R_{i+1/2,j} &= \mathbf{U}_{i+1,j} - \frac{s_{i+1,j}^L}{4} \left[ \left( 1 - \frac{s_{i+1,j}^L}{3} \right) A_{i+1,j}^i + \left( 1 + \frac{s_{i+1,j}^L}{3} \right) \nabla_{i+1,j} \right].
\end{align*}
\]

The forward and back difference operators are defined by, respectively,

\[
\begin{align*}
A_{i,j}^i &= \mathbf{U}_{i+1,j} - \mathbf{U}_{i,j}, \\
\nabla_{i,j} &= \mathbf{U}_{i,j} - \mathbf{U}_{i-1,j}.
\end{align*}
\]

The Van Albada limiter

\[
s_{i,j} = \frac{2A_{i,j}^i \nabla_{i,j}^i + \delta}{(A_{i,j}^i)^2 + (\nabla_{i,j}^i)^2 + \delta}
\]

is used to prevent overshoots and undershoots near discontinuities, where \( \delta \) is a very small positive number to prevent division by zero in regions of uniform flow.

A two-stage, second order Runge–Kutta scheme of Shu and Osher [24] is used to integrate Eq. (10) in time direction. After spatial discretization, Eq. (10) can be treated as a set of ordinary differential equations:
\[
\frac{d\mathbf{U}_{i,j}}{dt} = \mathbf{L}_{i,j}(\mathbf{U}),
\]
where
\[
\mathbf{L}_{i,j}(\mathbf{U}) = -\frac{1}{\Omega_{i,j}} \sum_{k=1}^{4} \sum_{m=1}^{N} (T_{k}^{m})^{-1} \hat{F}_{k}^{m} z_{k} \Delta l_{k}.
\]

Then this scheme is given by
\[
\mathbf{U}_{i,j}^{(0)} = \mathbf{U}_{i,j}',
\]
\[
\mathbf{U}_{i,j}^{(1)} = \mathbf{U}_{i,j}^{(0)} + \Delta t \mathbf{L}_{i,j}(\mathbf{U}^{(0)}),
\]
\[
\mathbf{U}_{i,j}^{(2)} = \frac{1}{2} \mathbf{U}_{i,j}^{(0)} + \frac{1}{2} (\mathbf{U}_{i,j}^{(1)} + \Delta t \mathbf{L}_{i,j}(\mathbf{U}^{(1)})),
\]
\[
\mathbf{U}_{i,j}^{n+1} = \mathbf{U}_{i,j}^{(2)}.
\]

### 3.5. Some remarks

Although the dissipation properties for genuinely non-linear fields are not studied (in this case it turns out to be very difficult to compare the numerical dissipations between the grid-aligned method and the rotated method), numerical tests indicated that the resolution to shock waves for the first order rotated FDS scheme is similar or slightly inferior to its grid-aligned counterpart. However, when a second order rotated scheme is used, it can capture shocks almost as accurate as the second order grid-aligned scheme and, furthermore, the shock instability can be suppressed completely.

Numerical experiments to be presented in the next section show that the rotated Roe scheme will not lead to entropy-violating solutions such as expansion shocks even without using any entropy fix procedure. This is possibly due to the increase of the numerical dissipations in the regions where non-physical solutions might be produced. However, in practice, the entropy fix of Huynh [11] is adopted to provide insurance against possible entropy-violating failings and this fix is applied to genuinely non-linear fields only.

It is obvious that the computational cost for the rotated Roe scheme is larger than that for the grid-aligned scheme since the Roe’s approximate Riemann solver has to be used twice on each cell interface. However, we can make the ratio of the CPU time between the rotated method and the grid-aligned methods less than 2 in evaluating the flux functions. This can be done due to the following facts:

1. The Roe-averaged quantities are only needed to compute once;
2. The strength of shear wave corresponding to \(n_1^k\) is zero;
3. The entropy wave eigenvectors corresponding to \(n_1^k\) and \(n_2^k\) are identical.

By taking these facts into consideration, we can implement the rotated Roe scheme efficiently and this CPU time ratio is about 1.5. In the three-dimensional case, this ratio can be even smaller...
because only seven out of ten waves need to be computed (in the two-dimensional case, six out of eight waves need to be computed). Furthermore, if the \(\varepsilon\) in Eq. (16) is suitably selected, the time needed for evaluating the rotated flux function can be further reduced because when

\[
\sqrt{(\Delta u_{i+1/2,j})^2 + (\Delta v_{i+1/2,j})^2} \leq \varepsilon
\]

is satisfied, we need only to evaluate \(U_{i+1/2,j}\) in a grid-aligned manner. Numerical tests indicate that the computational results are not sensitive to the value of \(\varepsilon\) unless it is too large. In this paper, \(\varepsilon\) is determined by

\[
\varepsilon = (10^{-3} - 10^{-5}) U^*,
\]

where \(U^*\) is the free stream velocity or velocity at inlet of the flow field. With \(\varepsilon\) determined by the above equation, we find that the condition \(\sqrt{(\Delta u_{i+1/2,j})^2 + (\Delta v_{i+1/2,j})^2} \leq \varepsilon\) is always satisfied except in the regions containing shock waves and strong compression/rarefaction waves where the velocity-differences are large. This makes the computational costs for the rotated Roe scheme comparable to its grid-aligned counterpart with H-type entropy fix [23] for many test cases.

4. Numerical tests

In this section, the rotated FDS scheme based on Roe’s approximate Riemann solver is used to solve four inviscid flow test cases. All the computational results are compared with those obtained by using the grid-aligned Roe scheme. For each test case, we take \(\gamma = 1.4\) and \(\varepsilon = 0.0001 U^*\). The first three test cases are computed using the first order scheme to show the shock stability property of the rotated Riemann solver. The time integration of the first order scheme is carried out by using forward Euler method. The last case is computed with the second order scheme that has been described in Section 3 to test the resolution of the higher order rotated FDS scheme. Except specifically mentioned, entropy fix of Huynh [11] is applied to both the grid-aligned and the rotated Riemann solvers. The time step is determined by

\[
\Delta t = \min_{i,j} \left( \frac{|\Omega_{i,j}|}{\beta_{13} + \beta_{24}} \right) \text{CFL},
\]

where

\[
\beta_{13} = \left( u_{i,j}(n_{x1} + n_{x3}) + v_{i,j}(n_{y1} + n_{y3}) \right)/2 + a_{i,j}(|\Delta l_1 n_1 + \Delta l_3 n_3|)/2,
\]

\[
\beta_{24} = \left( u_{i,j}(n_{x2} + n_{x4}) + v_{i,j}(n_{y2} + n_{y4}) \right)/2 + a_{i,j}(|\Delta l_2 n_2 + \Delta l_4 n_4|)/2.
\]

The CFL number for all test cases is chosen as 0.5.

4.1. Case 1. Odd–even grid perturbation problem

This test case has been reported in [19] and later investigated by several authors [5,15,18]. It is well known that many upwind schemes, including the exact Riemann solver by Godunov [7] and the approximate ones by Roe [20] and Osher and Solomon [17] are afflicted with the shock instability (also called odd–even decoupling). We use this case to investigate the performance of rotated Roe scheme with different upwind directions.
We consider a plane shock wave that propagates downstream in a straight duct at the speed of \( M_s = 6 \). This problem is computed on a grid of \( 800 \times 20 \) cells. Each cell is a square with unit side, except those on the centerline where the grid is perturbed in the following manner:

\[
y_{i,j_{mid}} = \begin{cases} 
  y_{i,j_{mid}} + 10^{-3} & \text{for } i \text{ even}, \\
  y_{i,j_{mid}} - 10^{-3} & \text{for } i \text{ odd}.
\end{cases}
\]

We note the magnitude of perturbation is the same as that in [18] and larger than that used in [19] to emphasize the problem of shock instability. The initial position of the shock wave is at \( x = 20 \).

To the right of the shock, the initial conditions are

\[
(\rho, u, v, p) = (1.4, 0, 0, 1).
\]

To the left of the shock, the flow variables are computed using moving shock relations. The left boundary is supersonic inflow boundary where all flow variables are prescribed using their initial values. At the right boundary, all gradients are set to zero. The top and bottom boundaries are solid walls where the reflecting boundary condition is used. Fig. 5a shows the predicted density contours using first order grid-aligned Roe scheme and Fig. 5b–e show the density contours using first order rotated Roe schemes with the upwind directions determined by velocity vector, pressure gradient, velocity-magnitude gradient and velocity-difference vector respectively. All figures show the captured shock waves at \( t = 100 \). For the grid-aligned FDS scheme, the shock has broken down completely because of the odd–even decoupling promoted by the perturbation to the grid centerline. When using the velocity vector to compute the upwind direction, the rotated FDS scheme also leads to a shock-unstable solution similar to the grid-aligned scheme. This is expected since during the development of the disturbance, the flow direction is almost grid-aligned and the rotated FDS scheme is almost identical to the grid-aligned one. The use of the gradient of certain flow quantity as the upwind direction can attenuate the shock instability. As being depicted in Fig. 5c and d, the disturbances that are induced on the centerline remain confined in the numerical shock layers because in these cases the rotated FDS schemes are almost grid-aligned only inside or adjacent to the shock layers. It is seen from Fig. 5e that the odd–even decoupling phenomenon is removed completely by using the velocity-difference vector as the upwind direction. We note that among all quantities for determining the upwind direction, only the velocity-difference vector can be considered as a measurement for the spatial fluctuations of the numerical solution inside and along the numerical shock layer. This fact is crucial for the rotated FDS scheme to be shock stable and seems to support the heuristic explanation of the shock instability given in [29]. In what follows, we only use the velocity-difference vector to determine the direction of upwinding. Fig. 6a and b show the density contours at \( t = 300 \) and \( t = 600 \) respectively using the first order rotated Roe scheme. It can be seen that the proposed rotated FDS scheme remains to be shock stable for sufficiently long time.

4.2. Case 2. Inviscid supersonic flow (\( M_\infty = 20 \)) around a circular cylinder

This is another well-known test case to examine the catastrophic carbuncle failings of some Riemann-solver-based FDS scheme. The free stream Mach number is 20 [18], and this test problem is computed on a grid with 20 cells in the radial direction and 720 cells in the circumferential direction with the first order grid-aligned Roe scheme and the first order rotated Roe
Fig. 5. The odd–even grid perturbation problem (density contours). The numerical results are computed with (a) the grid-aligned Roe scheme, (b) the rotated Roe scheme with $\mathbf{n}_t$ determined by velocity vector, (c) pressure gradient, (d) velocity-magnitude gradient and (e) velocity-difference vector. The total number of time steps for each computation is (a) 2527, (b) 2541, (c) 2112, (d) 2111 and (e) 2111.
scheme. The boundary conditions used in this paper are similar to those used in [18]. The very elongated mesh in the radial direction will initiate the so-called carbuncle phenomenon when using the grid-aligned FDS scheme as shown in Fig. 7a. On the other hand, the numerical result of rotated FDS scheme shown in Fig. 7b does not exhibit such kind of shock instability. For the grid-aligned scheme, the steady state solution is obtained after 30,000 iterations with 
\[
\|\rho^{n+1} - \rho^n\|_1 \leq 10^{-7}
\]
when the single precision arithmetic is used. For the rotated FDS scheme, the steady state solution can be also obtained. But after about 11,000 iterations, the residual stagnates at 
\[
\|\rho^{n+1} - \rho^n\|_1 \approx 3.5 \times 10^{-5}
\]
and will not decrease further.

4.3. Case 3. The diffraction of a supersonic shock moving over a 90° corner

The shock Mach number is 5.09. The computational domain is a unit square \([0, 1] \times [0, 1]\) that is discretized into a \(400 \times 400\) uniform cells. The corner is at \((x, y) = (0.05, 0.625)\). Initially, the shock is at \(x = 0.05\). To the right of the shock, the flow field is initialized to
\[
(\rho, u, v, p) = (1.4, 0, 0, 1).
\]
To the left of the shock, the flow variables are computed using moving shock relations. At the left, right, and bottom boundary, all flow quantities are prescribed. At the top, time-dependent conditions determined by the exact motion of the shock are used. The solid walls are treated using the reflecting boundary condition. Quirk [19] has shown the complexity of the flow using a very fine grid to resolve the details of the flow field structures. He pointed out that some Riemann solvers encountered difficulties on a fine mesh and thus placed an upper limit on the resolution of simulations. Fig. 8a shows the density contours obtained by using the first order grid-aligned Roe scheme at \(t = 0.1561\). By using entropy fix, the grid-aligned FDS scheme can overcome the
expansion fan at the corner. However, the shock instability again appears after the moving planar shock. Fig. 8b displays the numerical result obtained by the first order rotated FDS scheme on the same grid and at the same time. It can be seen the shock can be sharply captured with a resolution similar to the grid-aligned scheme without any anomaly. Next, we re-compute the same case with the entropy fix being turned off for both the first order grid-aligned Roe scheme and the first order rotated Roe scheme. The numerical results are shown in Fig. 9a and b respectively. In Fig. 9a, besides the shock instability, the grid-aligned Roe scheme gives rise to a near discontinuous expansion fan near the corner as it is expected. But when comparing Fig. 9b with Fig. 8b, it can be seen that the rotated Roe schemes with and without entropy fix give virtually the same results. Although no general conclusion can be given, it seems that the entropy fix is not needed by the rotated FDS schemes for some test cases.

4.4. Case 4. Mach 3 wind tunnel with a step

This problem was first proposed by Woodward and Colella [30]. The computational domain is \([0, 3] \times [0, 1]\). The corner of the step is located at \((x, y) = (0.6, 0.2)\). The initial conditions are 

\[(\rho, u, v, p) = (1.4, 3, 0, 1).\]
All flow variables are fixed at the left boundary. At the right boundary, all gradients are set to zero. The symmetry condition is used at the bottom boundary to the left of the step. Other boundaries are solid walls where the reflecting condition is used. The computation is carried out on a uniform mesh with $200 \times 80$ cells using second order grid-aligned and rotated Roe schemes. The special treatment proposed in [30] is used near the corner. The grid size is $\Delta x = \Delta y = 1/80$.

Fig. 8. The diffraction of a supersonic shock moving over a $90^\circ$ corner (density contours). The numerical results are obtained with (a) the first order grid-aligned Roe scheme with entropy fix and (b) the first order rotated Roe scheme with entropy fix. The total number of time steps for each computation is (a) 897 and (b) 873.
and the computed density contours corresponding to these two schemes at $t = 4.0$ are shown in Fig. 10a and b respectively. Even in this case, the grid-aligned Roe scheme exhibits instability in regions after the normal shock (however, on a coarser grid with $120 \times 40$ cells, this instability cannot be observed clearly). In contrast, the rotated FDS scheme again demonstrates a robust shock-capturing capability. The shock waves can be captured in high resolution without showing any instability. Fig. 11 reports $\mathbf{n}_{i+1/2,j}$, the normalized unit vectors that stand for the upwind
directions on the vertical faces of the cells. One should note that these vectors are drawn for every other cell face in each direction and only for the cell faces satisfying the condition \[ (\Delta u_{i+1/2,j})^2 + (\Delta v_{i+1/2,j})^2 \geq \varepsilon. \] It is evident that the upwind directions align normal to the bow shock and reflected shocks quite well. We can observe that the velocity-difference is larger than \( \varepsilon \)

---

Fig. 10. Mach 3 wind tunnel with a step (density contours). The numerical results are obtained with (a) the grid-aligned Roe scheme and (b) the rotated Roe scheme with \( \mathbf{n}^i \) determined by the velocity-difference vector. The total number of time steps for each computation is (a) 3966 and (b) 3960.

---

Fig. 11. Mach 3 wind tunnel with a step. The upwind directions \( (\mathbf{n}^i_{i+1/2,j}) \) are plotted for every other cell face in each direction and only for the cell faces satisfying the condition \[ \sqrt{(\Delta u_{i+1/2,j})^2 + (\Delta v_{i+1/2,j})^2} \geq \varepsilon. \]
on only small part of the cell faces. Therefore, the rotated FDS code can run very efficiently in this test case. In fact, this observation is also true for other test cases in this section although it has not been mentioned therein.

5. Concluding remarks

In this paper, a robust shock-capturing scheme is proposed based on the rotated Roe’s approximate Riemann solver. When the upwind direction is determined by the velocity-difference vector, the rotated FDS scheme demonstrates a robust shock-capturing capability and the shock instabilities or carbuncle phenomenon can be eliminated completely. The dissipation property associated with the linear field of the rotated FDS scheme is analyzed, and it is found that the rotated FDS scheme automatically introduces artificial dissipation in regions where some control of the shock instability is required. Furthermore, the proposed scheme can compute the grid-aligned shear waves (or boundary layers in viscous flows) as accurately as the grid-aligned FDS scheme, since it essentially reduces to the grid-aligned FDS scheme for such problems. Although it is needed to run the Roe’s approximate Riemann solver twice on every cell interface, the rotated FDS method can be implemented efficiently by taking several features of this method into consideration.

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References
